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AIAA 2000-2430

INFLUENCE OF GAS-SURFACE INTERACTION MODELS ON PREDICTED PERFORMANCE OF A MICRO-RESISTOJET

Andrew D. Ketsdever[†]
Air Force Research Laboratory
Propulsion Directorate
Edwards AFB, California

Dean C. Wadsworth[*]
ERC, Inc.
Edwards AFB, California

E.P. Muntz[‡]
University of Southern California
Department of Aerospace Engineering
Los Angeles, California

ABSTRACT

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The Free Molecule Micro-Resistojet was designed as a micropropulsion system capable of performing attitude control and primary maneuvers for nanospacecraft with a mass less than 10 kg. The details of gas-surface interactions between propellant molecules and surfaces held at elevated temperature are critical in predicting the propulsion system's performance and efficiency. The aim of this study is to assess parametrically the performance of a typical thruster geometry using a general Maxwell scattering model and two versions of the Cercignani-Lampis-Lord model. The models are incorporated into a Direct Simulation Monte Carlo numerical code and are used to bound the predicted performance characteristics of the thruster. The total specific impulse varies by approximately 20% over range of accommodation coefficients from specular to diffuse surface scattering. However, there was only a maximum difference of about 5% between the models for a given accommodation coefficient. Other more microscopic parameters, such as axial velocity distribution functions, appear to depend more on the scattering model used.

[†] Senior Research Engineer, Advanced Concepts Division, Senior Member.
andrew.ketsdever@ple.af.mil
[*] Research Scientist, Member.
[‡] A.B. Freeman Professor, Department Chair, Fellow.

INTRODUCTION

The Free Molecule Micro-Resistojet (FMMR) has been designed and developed as a primary and attitude control thruster for nanospacecraft ($m \leq 10$ kg).[1,2] The FMMR is constructed using microelectromechanical systems (MEMS) fabrication techniques which allows it to be machined on a micrometer scale and to be easily integrated with other MEMS components such as embedded control systems, valves, and pressure regulators. Although MEMS fabrication can be very beneficial to micropropulsion systems, a serious drawback of traditional MEMS micromachining is that only compatible materials can be used in the fabrication process which can limit device performance. A schematic of the FMMR is illustrated in Figure 1.

The propellant gas enters into the FMMR stagnation region through a MEMS valve and filter assembly connected by the propellant inlets. The device operates at unusually low pressures (50 – 500 Pa) which gives the propellant gas molecules a mean free path on the order of the expansion slot width. With MEMS fabrication techniques, the slot size can be machined with a width as small as ~ 1 μm; however, the nominal FMMR slot geometry used in this study has a slot width ~~$w \neq$~~ 100 μm. Energy is imparted to the propellant gas through collisions with a thin film heating element suspended above a silicon pedestal. The pedestal~~s~~ acts to minimize direct line-of-sight propellant transport through an expansion slot after entering the stagnation region.

The design requirement is to arrange a surface held at the required temperature to be the last surface contacted by a propellant molecule before it exits the device through an expansion slot. This requirement suggests that the spacing between the thin film heater and the expansion slot be on the order of the molecular mean free path in the device to reduce intermolecular collisions before expansion.

The FMMR relies on the transfer of energy into a propellant gas through molecular collisions with the heated surface. Since the thin film heater is the only heated surface in the device, subsequent molecular collisions with relatively cold thruster surfaces is expected to be a major loss mechanism. For these reasons, the details of the gas-surface interaction are critical in predicting the propulsion system's performance and efficiency. The aim of this study is to assess parametrically the performance (thrust and specific impulse) of a typical FMMR geometry using several gas-surface interaction models. The models are incorporated into a Direct Simulation Monte Carlo (DSMC)[3] code to bound the predicted performance characteristics of the thruster.

THEORY

In a uniform free molecule flow, the thrust $\Im$, or flux of normal momentum, produced by a gas at a stagnation pressure of p_o through a thin orifice or slot of area A_o is

$$\Im = \frac{p_o}{2} A_o = \frac{n_o k T_o}{2} A_o \qquad (1)$$

where n_o and T_o are the number density and temperature in the stagnation region. In the case of the FMMR, the stagnation temperature in the vicinity of the expansion slot is governed by the physics of the interaction between the propellant gas and the thin film heated element. For the present study, the thin film heated element is assumed to be an inert surface material defined by a wall temperature T_w and a single energy accommodation coefficient a. Therefore,

$$T_o = aT_w + (1-a)T_i \qquad (2)$$

In the case of the FMMR, the stagnation temperature is in the vicinity near the expansion slot, and T_i is the temperature of the molecules at the propellant inlet of the thruster. The free molecule mass flow through the orifice or slot is

$$\dot{m} = m\frac{n_o \overline{c'}}{4} A_o = \frac{m n_o}{4}\sqrt{\frac{8kT_o}{\pi m}} A_o \qquad (3)$$

where m is the propellant molecular mass, and $\overline{c'}$ is the average thermal speed of the gas.

A propulsion system's efficiency is generally evaluated based on the thruster's intrinsic specific impulse or I_{sp}. The I_{sp} of a propulsion system is the ratio of the thrust generated to the propellant mass flow required to produce the thrust. For a free molecule flow through a thin orifice or slot the specific impulse is given by

$$I_{sp} = \frac{\sqrt{\frac{\pi k T_o}{2m}}}{g_o} \qquad (4)$$

where g_o is the gravitational constant. As evident in the above formulation, the details of the energy exchange between the thin film heaters and propellant molecules drive the performance of the FMMR.

CALCULATIONS

The analytical, free molecule results from the previous section are expected to be useful in the basic design of the FMMR; however, ~~Direct Simulation Monte Carlo (~~DSMC~~)[3]~~ calculations already defined are required to predict flowfield properties of the actual FMMR under transitional rarefied gas conditions. Many of the input models required, such as gas-surface interaction, are topics of current research. Parametric variation of the model features can be used to assess performance sensitivity to these uncertainties independently.

The two-dimensional computational domain for are the nominal FMMR geometry is shown in Fig. 2. The geometry is symmetrical about the slot centerline IJ. Boundary AB is an open inlet; molecules entering are selected from a drifting equilibrium distribution at T_i, with the drift velocity iteratively updated to match the input plenum pressure at the boundary. Boundary CD is a plane of symmetry (assuming a multi-slot configuration). The farfield vacuum boundary DJ is placed approximately 10 slot widths downstream of the slot exit. Each wall surface is a reflector defined by an accommodation coefficient a and an input temperature, either T_I or T_w (surface FI only).

The key feature that enhances bulk flow in the propellant gas is the differential heating of the thin film heater FI (at T_w) relative to that of the nominal plenum inlet and surface temperature (at T_i). In this study, all surfaces except the thin film heater are assumed to be at the gas inlet temperature T_i. More accurate simulations, which iteratively couple the gas and structural heat transfer properties and thus eliminate the need for an input surface temperature distribution, will be reported at a later time.

The code is instrumented to directly sample and spatially resolve the flux of molecular mass, momentum, and energy through an arbitrary flowfield plane, here typically chosen to be the slot throat (GG') or the slot exit (HH'). The code also samples the axial and transverse velocity distribution function at arbitrary locations, including surface boundaries, to allow more detailed comparison with the simple free molecule theory. In this manner, performance losses can be attributed to various components of the geometry such as the slot walls GH.

For the present highly rarefied operating conditions, the DSMC requirement that the nominal cell size be on the order of the local molecular mean free path and that the simulation timestep be small relative to the mean collsion time are easily met. The nominal simulation grid contained 2000 cells, with cell sized to be typically much less than 25% of the local mean free path. The nominal timestep was approximately 50% of the collision frequency.

The simulations were run for 2000 unsteady and 10^4 additional steady-state timesteps during which sampling of the flowfield occurred. The nominal simulation contained 2×10^5 particles at steady state. Statistical scatter in the predicted specific impulse is estimated to be much less than one percent due to the large sample sizes obtained.

For simplicity in these initial design studies, calculations have been made assuming an argon propellant, although it is far from an optimum choice for an electrothermal thruster. The typical propellant inlet temperature and pressure are 300 K and 50 Pa, respectively. The nominal FMMR geometry has a slot width of w = 100 μm, an expansion angle α = °40 and an ? delete comma expansion slot thickness of 250 μm. The inlet conditions and slot width yield a Knudsen number of unity.

GAS-SURFACE INTERACTION MODELING

Despite advances in micromachining technology, silicon and silicon-based materials are still the most common material used in MEMS fabrication. Exposure of pure silicon to potential propellant gases such as ammonia (NH_3) or water (H_2O) will lead to dissociative adsorption and subsequent nitridation or oxidation of the silicon surface even under benign conditions (e.g. room temperature).[4] Very little information is available regarding their influence on macroscopic processes such as gas transport.[5] Molecular-level data indicate desorption is, in general, a highly non-equilibrium process,[6] further complicating model development.

As such for the present performance studies, an inert surface material defined by a wall temperature T_w or T_i and a single accommodation coefficient a are assumed. An estimate of the influence of the reflection (or desorption) process on overall performance is then made by comparative calculations for three models: the Maxwell model,[3] and two forms of the Cercignani-Lampis-Lord (CLL) model.[7,8]

In the Maxwell model, a fraction a of incident particles fully accommodate to the wall temperature and are diffusely reflected with the remainder being specularly reflected. Molecular beam studies have shown that this model is not realistic, and that, in general, reflected molecules at a surface exhibit a lobular distribution in direction and a continuous spread in energy.

In the original form of the CLL model, reflection varies from specular (a = 0) to fully accommodating (a = 1) as with the Maxwell model.[7] However, the CLL original model allows for separate normal and tangential energy accommodation coefficients (which for simplicity are equivalent in this study). This form of the CLL model produces physically reasonable distributions of direction and energy for reflected molecules although it can not be used to describe discrete internal energy states of the molecule.

A generalized form provides for diffuse molecular reflection at a surface with incomplete energy accommodation.[8] This CLL diffuse model retains the energy distribution obtained from the original CLL model but chooses new polar and azimuthal scattering angles corresponding to diffuse reflection. Both the CLL original and CLL diffuse models are compared to the simple Maxwell model to assess the predicted FMMR performance.

In principle, the details of the energy deposition and desorption process can be directly incorporated into the DSMC gas-surface interaction procedure as they become available. For the present range of FMMR conditions, gas-phase processes such as recombination are negligible due to the low operating pressures. Therefore, the key parameters required for more detailed studies are the net velocities or translational energy components of the (potentially dissociated) products of the desorbing propellant molecule, rather than the specifics of the pathways by which the adsorption and decomposition occur.

THERMAL ACCOMMODATION OF GASES ON SURFACES

An extensive literature exists detailing the measurements of the thermal accommodation coefficient made for various gas-surface systems.[9-12] Although there have been a number of notable measurements made for monatomic or simple diatomic gases interacting with pristine metal surfaces, obtaining measurements and developing numerical models for complex flows on engineering surfaces is an area of active research.[13-16]

For the analysis presented here, the FMMR is operating on an argon propellant for simplicity. With current MEMS fabrication practices, the thin film heating element can either be made from a polysilicon material or sputter deposited metals such as platinum or gold. It is assumed for the purposes of this research that the heating element is a deposited platinum surface with a thickness of approximately 2000 Å.

The temperature dependent accommodation coefficient depends on several factors including the physical characteristics of the gas, the solid surface, the surface temperature, and the gas temperature. From previous research, the accommodation coefficient for argon impacting a platinum surface ranges from 0.71[9] to 0.9[11] at T_w = 300 K. At the FMMR operating temperature of T_w = 600 K, the accommodation coefficient ranges from 0.5[10] to 0.63.[11] There is no available data for the accommodation coefficients of argon colliding with a silicon surface which is required to estimate the energy losses on the expansion walls.

Due to uncertainties in the measurements and in some cases a complete lack of data, the calculations presented in the following section include full parameteric analysis with the accommodation coefficient. For simplicity, the accommodation coefficients of a given case are assumed to be equivalent for both the thin film heater and the expansion walls. In light of these difficulties, the experimentally derived accommodation coefficients can be used as a general guideline in assessing predicted FMMR performance.

RESULTS

Baseline estimates of the FMMR performance (i.e. thrust and specific impulse) and flowfield behavior were obtained assuming a Maxwell surface model with complete accommodation (a keep "a" (=1). At this condition, the Maxwell and both versions of the CLL model are equivalent. stet ~~Figure~~ 3 shows the FMMR flowfield contours for complete surface accommodation with T_w = 600 K. The contours consist of raw data with translational temperature on the left side and axial velocity on the right side. At this level of rarefaction (Kn ~ 1), slip phenomena is expected to be significant as confirmed by the peak temperature in the gas near the heated surface remaining much lower than T_w. Figure 4 compares the calculated specific impulse with the theoretical value (Eq. 4) as a function of the heated wall temperature. For the nominal case, the corresponding thrust per unit expansion slot length is nearly 2.5 mN/m.

Figure 5 shows the centerline axial velocity distribution function at the expansion slot exit (H' in Fig. 2) and throat (G' in Fig. 2) for the nominal case using the Maxwell model with a = 1. Also shown are the theoretical half-Maxwellian free molecule distributions evaluated at T_w and T_i. The theoretical free molecule axial velocity distribution function would consist of a half-Maxwellian at T_w. Obviously, the flowfield at the exit differs from the simple free molecule analysis; however, the comparisons in Fig. 4 suggest that they can serve well for initial performance studies.

Figure 6 shows the net axial force along the expansion slot walls for various expansion angles α. For these results, the heated wall temperature is $T_w = 600$ K and the expansion slot wall temperature is $T_i = 300$ K with full surface accommodation. The net increase or decrease in thrust contributed by the expansion walls is given by the integrals under the curve in the figure. For smaller expansion angles ($\alpha = 40°$ or 54.74°), the expansion walls contribute a net positive increment to performance by limiting divergence losses. It is interesting to note that the enhancement reaches a maximum midway along the expansion indicating that thin expansion slots are preferred. As the expansion angle increases for a fixed slot thickness, the shear forces begin to dominate and can significantly degrade the thruster's performance. From this analysis, relatively thin expansion walls with expansion angles $\alpha \leq 60°$ are desirable.

As mentioned earlier, the characteristics of the FMMR flowfield and performance are expected to depend on the details of the gas-surface interaction process. Figure 7 shows the specific impulse of the FMMR as a function of the surface accommodation coefficient for the Maxwell and the two versions of the CLL model. The models differ by only a few percent at a given accommodation. The accommodation coefficient in this case is assumed to be independent of the heated surface temperature; with this assumption, the peak specific impulse occurs for a = 1. The difference between the results from the DSMC incorporated models and the free molecule theory lies in the effects of the expansion slot walls on the FMMR performance. As indicated in Fig. 6, the expansion slot walls act to improve the performance for small expansion angles. Since the free molecule theory is only truly valid for an infinitely thin orifice expansion, the effect of the slot walls is not accounted for in the theoretical results shown in Fig. 7.

Normalized specific impulse profiles across the slot expansion exit plane (HH' in Fig. 2) for various conditions are shown in Fig. 8. As expected, the maximum specific impulse contribution is on the FMMR centerline where losses due to the transverse velocity and collisions with the expansion walls are minimized. The specific impulse drops approximately 30% from the centerline value as the expansion walls are approached. Interestingly, it appears that the nature of the scattering process has a larger affect on the profile shape that the magnitude of the accommodation.

Figure 9 shows the influence of the model on the net axial force along the expansion slot wall for $\alpha = 40°$. This effect is larger than that due to modest variations in the expansion slot angle about the nominal value shown in Fig. 6. Figure 9 also indicates that the scattering process contributes significantly to the determination of the optimal slot expansion length. To minimize shear and heat transfer to the expansion slot, thin expansion slots are desired. However, the benefit of re-directing errant molecules in the useful thrust direction is improved for longer slots.

The FMMR flowfield temperature contours for full accommodation and for the CLL diffuse model with a = 0.5 are shown in Fig. 10. As expected, the temperature profile near the heated wall surface shows less energy is transferred into the propellant gas under incomplete accommodation conditions.

The major performance loss mechanism is expected to be due to heated propellant molecules colliding with relatively cold thruster walls, particularly in the expansion region. Figure 11 shows the propellant heat flux as a function of axial distance along the FMMR expansion slot. The entrance of the slot (i.e. position closest to the heated wall) is denoted as x/w = 0. Figure 11 shows that there is little deviation between the gas-surface interaction models for a given accommodation indicating that the heat flux is relatively insensitive to the scattering model assumption. As expected, the heat flux to the expansion walls varies linearly with accommodation coefficient as shown in Fig.ure 12. For example, the numerical solution for a = 0.5 shows approximately one-half of the heat flux that a = 1.0 indicates.

DISCUSSION

As shown in Fig.ure 7, the details of the gas-surface interaction are important in effectively determining the predicted performance of the FMMR. As more appropriate propellants are investigated such as water vapor,[1] the physics of surface interactions will become increasingly complicated by adsorption, dissociation and internal energy state excitation. Currently, adequate models are not available to address these interactions.

The mass of propellant required to perform a series of orbital maneuvers is given by

$$m_p = m_i\left(e^{\frac{\Delta v}{I_{sp}g_o}} - 1\right) \tag{5}$$

where m_i is the dry spacecraft mass (i.e. without propellant) and Δv is the change in velocity that the propulsive maneuvers afford. A Δv of approximately 100 m/sec is typical for a nanospacecraft mission (m_i = 10 kg) where the micropropulsion system is used for attitude control over the mission lifetime. Figure 13 shows the propellant mass required for the assumption above over the range of FMMR predicted I_{sp} (Fig. 7).

As Eq. (5) indicates, an error in estimating the specific impulse can lead to larger errors in predicting the required propellant mass for a spacecraft mission due to the exponential term. For this reason, improved gas-surface interaction models and validating data are required to accurately estimate mission parameters.

CONCLUSIONS

It has been shown that the predicted performance of the FMMR depends on the details of the gas-surface interaction process used in the numerical scheme. In general, the macroscopic properties of the FMMR (specific impulse, expansion slot axial force and heat flux) appear to be more sensitive to the accommodation coefficient assumed than the details of the surface scattering. The total I_{sp} varies by approximately 20% over range of accommodation coefficients from specular (a = 0) to diffuse (a = 1) surface scattering. However, there was only a maximum difference of about 5% between the models for a given accommodation coefficient. Other more microscopic parameters, such as axial velocity distribution functions, appear to depend more on the scattering model assumption.

The performance of the FMMR, for a given accommodation on all surfaces, is maximized for a = 1 as shown by the numerical results. Performance may be further optimized by using a thin film heater material that fully accommodates while choosing a more specular surface for the expansion slots. This will allow for maximum energy input into the gas from the heating element and minimize the energy lost on the expansion walls.

Additional data is needed to assess the accommodation coefficient of gases on MEMS engineering surfaces such as silicon (single and polycrystalline), silicon oxide, silicon nitride, silicon carbide, and certain polymers. More physical gas-surface interaction models are required for FMMR calculations which simulate ideal propellants (typically stored as liquid) interacting with surfaces at elevated temperature. The details of molecular scattering, adsorption (physi- and chemi-), desorption, dissociation and internal energy mode coupling must be addressed.

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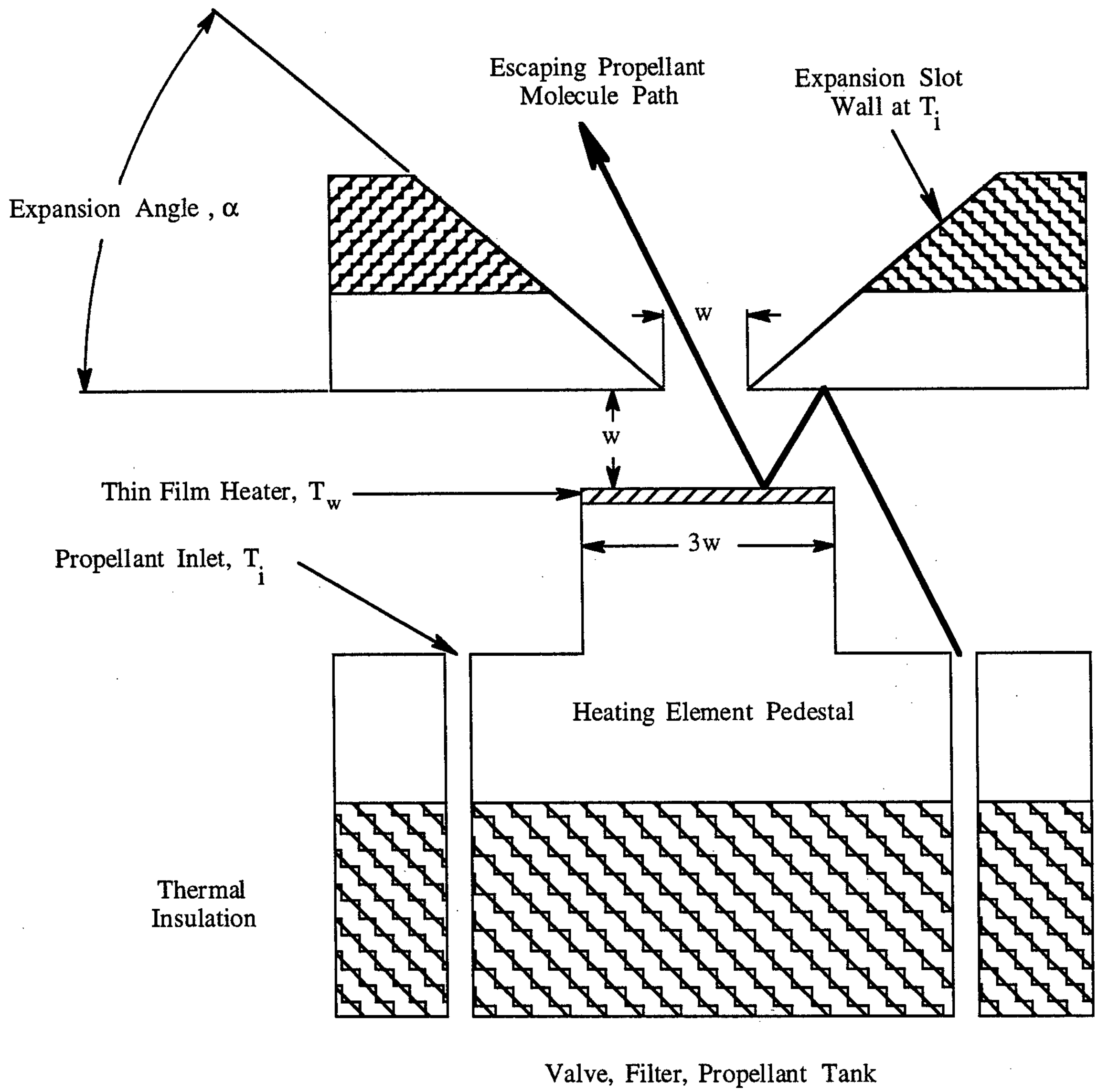
Escaping Propellant Molecule Path
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Heating Element Pedestal
Thermal Insulation
Valve, Filter, Propellant Tank

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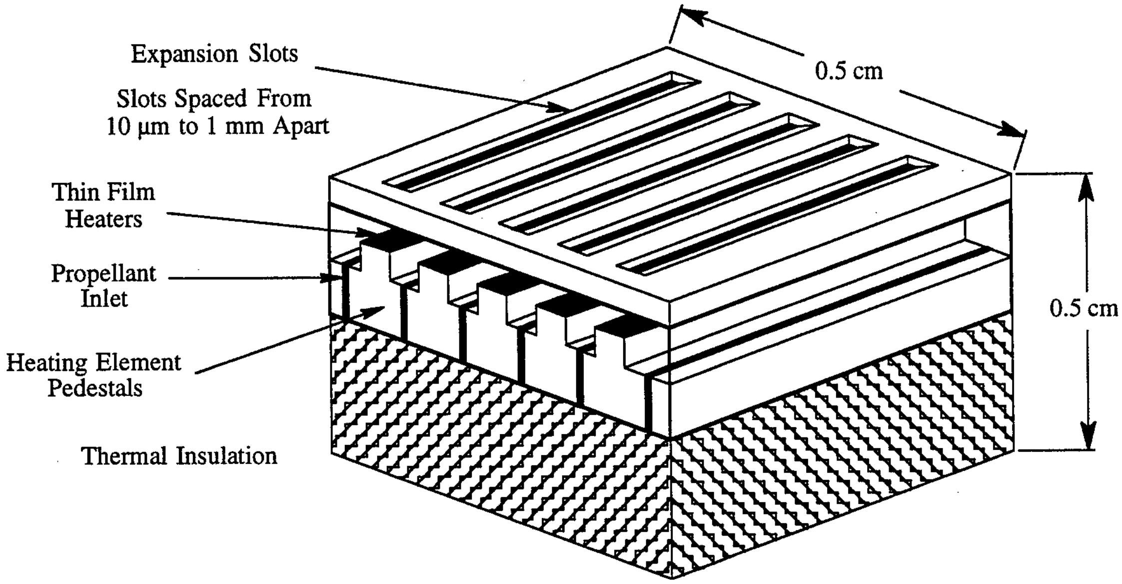
Fig 1.



FMMR Mounted Directly
to Valve, Filter and
Propellant Supply

Fig. 2

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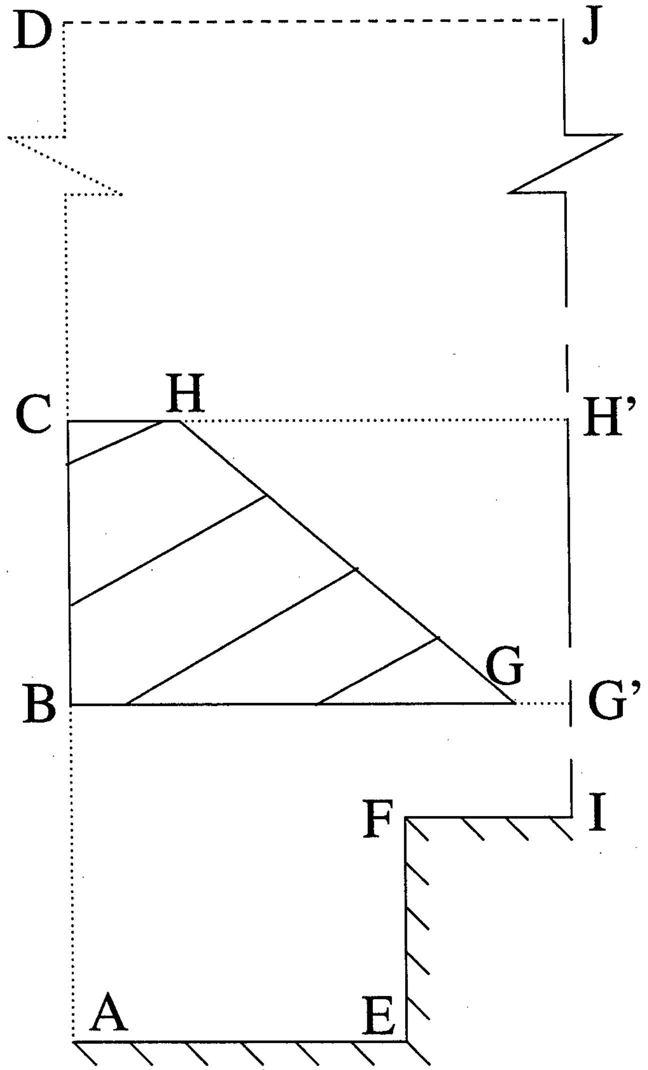

Fig. 3

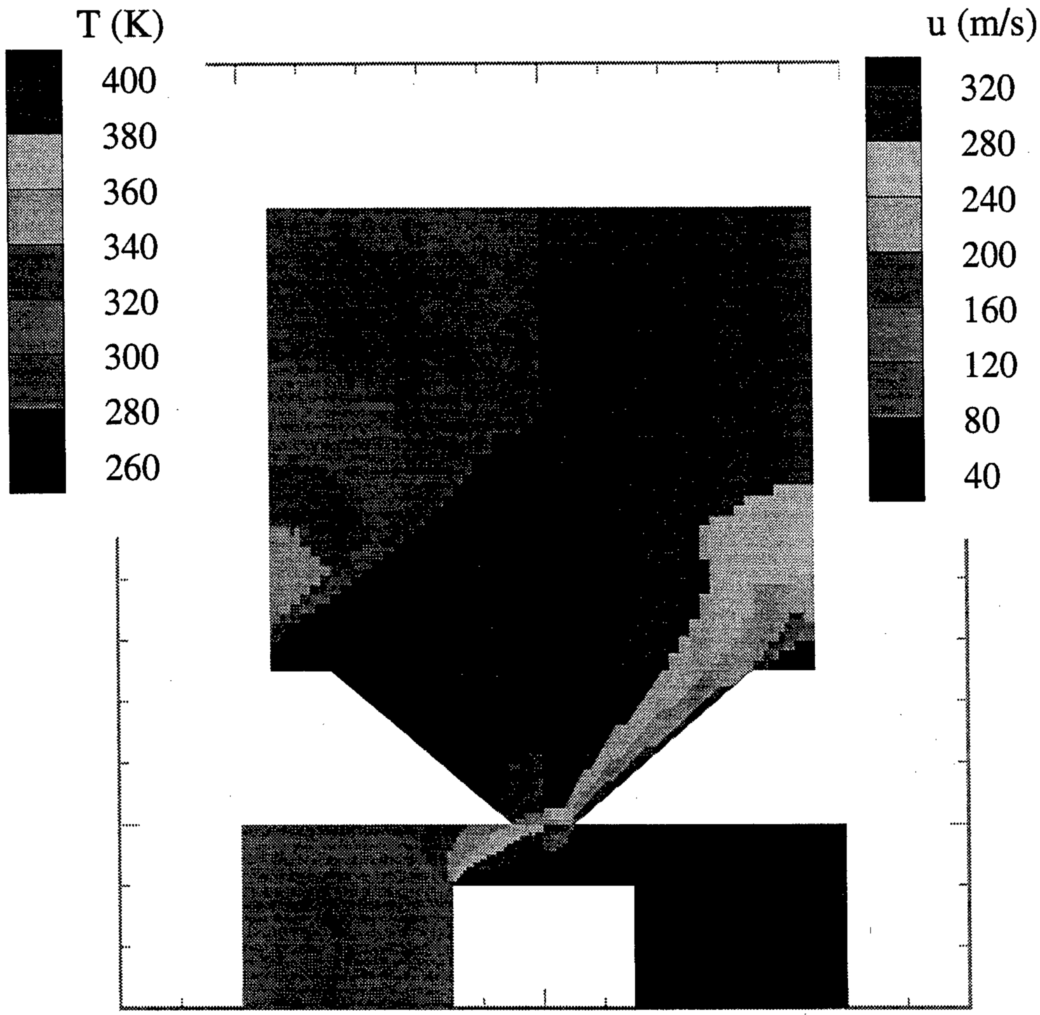
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Fig. 4

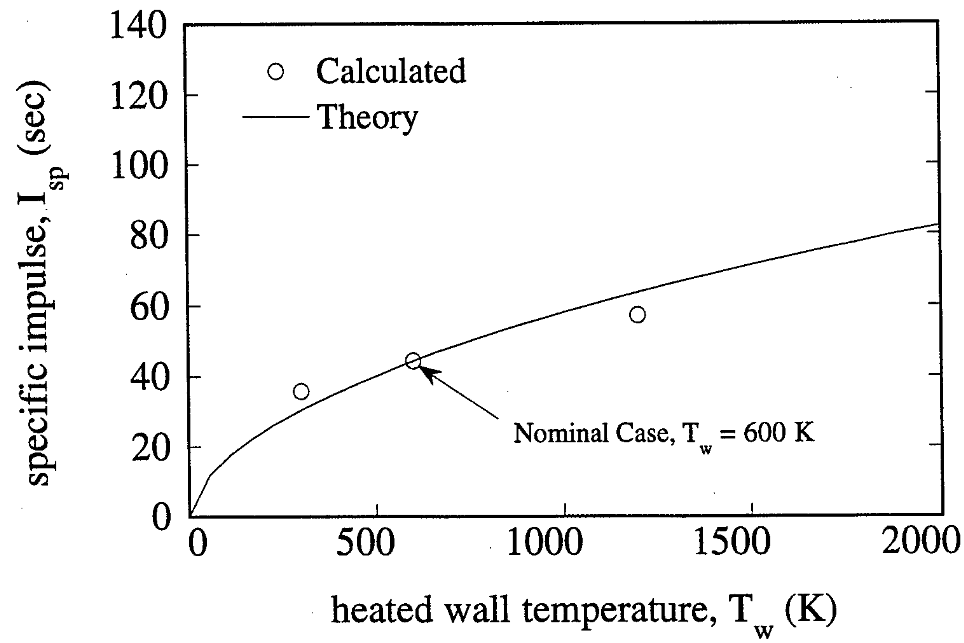

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Fig.5.

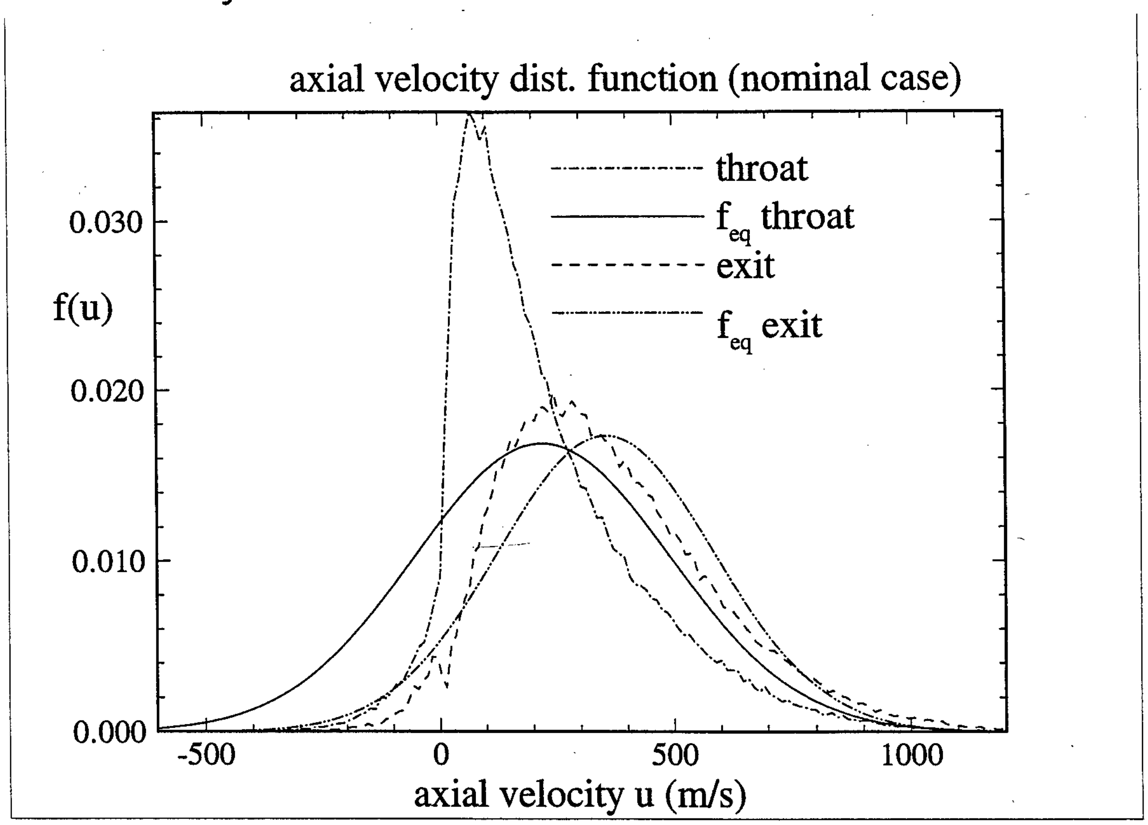

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Fig. 6

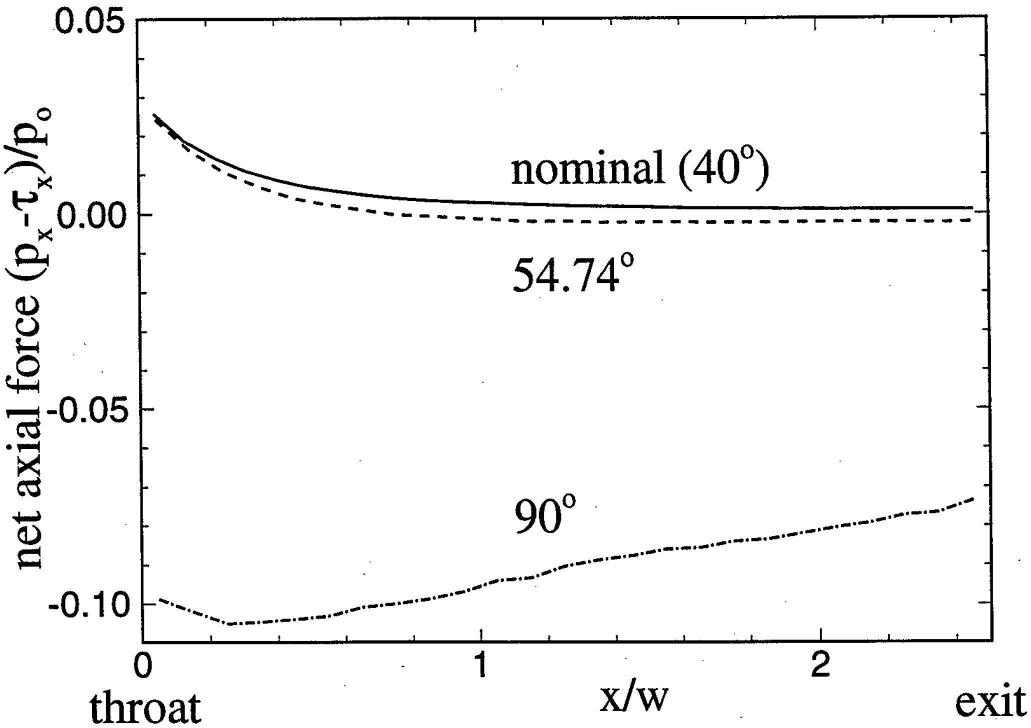
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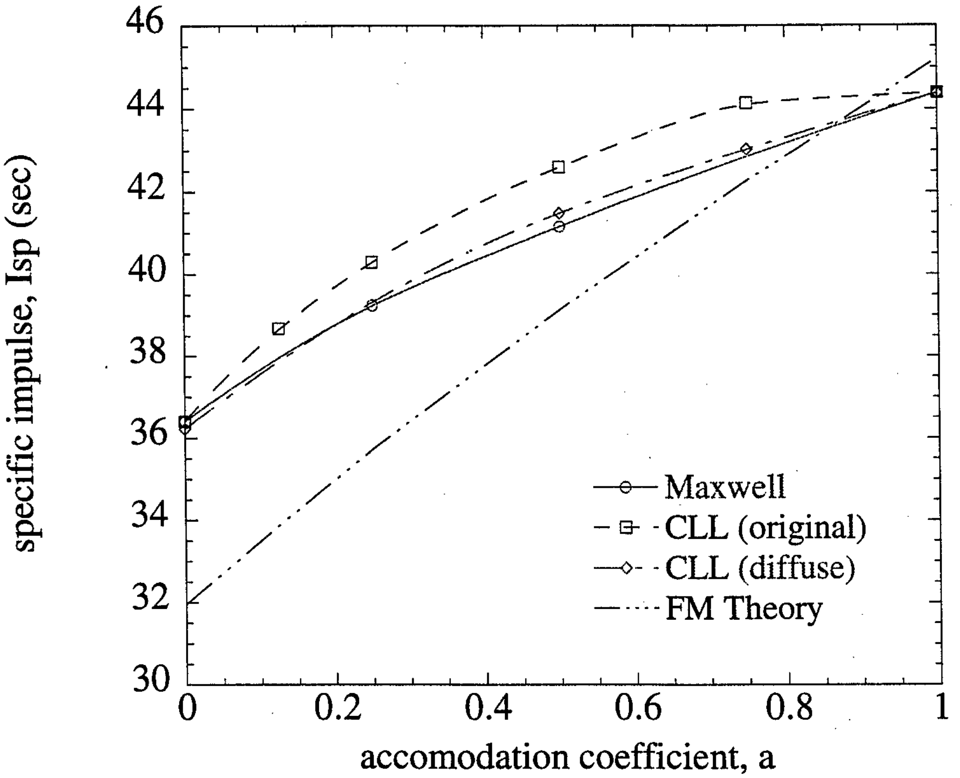
Fig. 7



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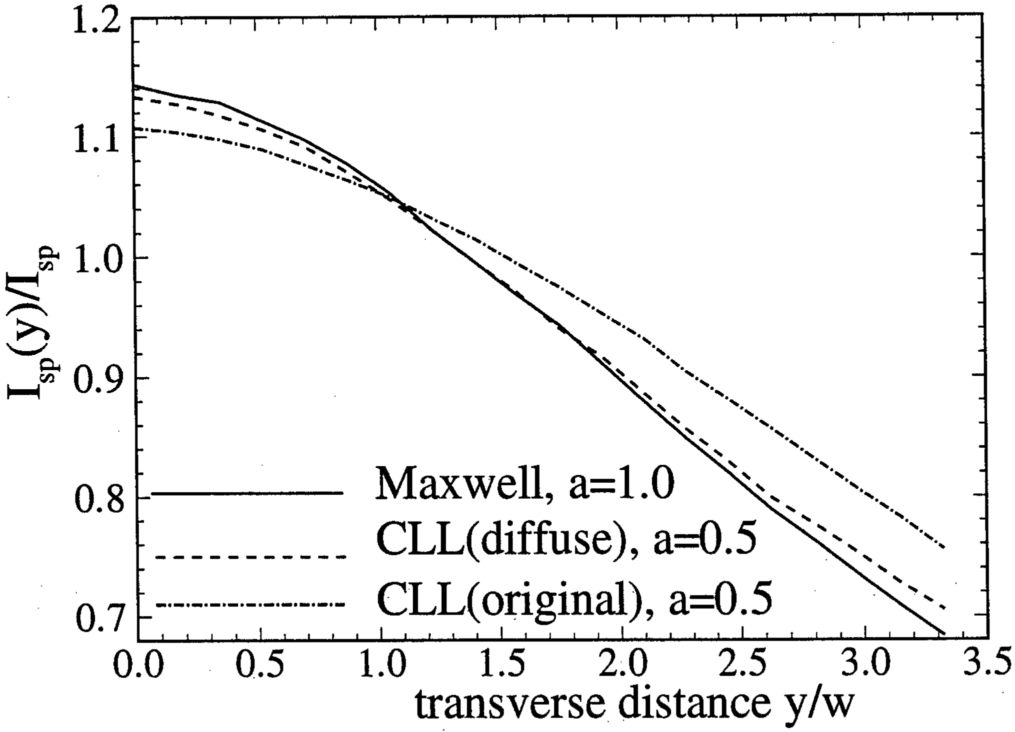
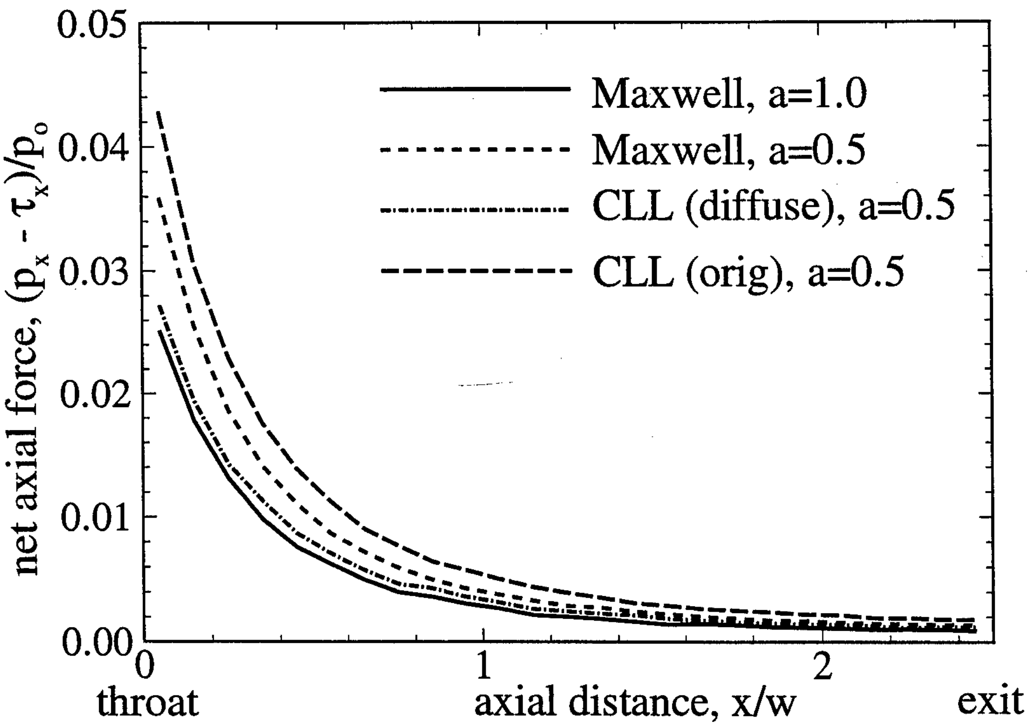
0.4
0.6
0.8
1
specific impulse, Isp (sec)
accomodation coefficient, a
Maxwell
CLL (original)
CLL (diffuse)
FM Theory

Fig. 8



1.2
1.1
1.0
0.9
0.8
0.7
$I_{sp}(y)/I_{sp}$
0.0
0.5
1.0
1.5
2.0
2.5
3.0
3.5
transverse distance y/w
Maxwell, a=1.0
CLL(diffuse), a=0.5
CLL(original), a=0.5

Fig. 9



0.05
0.04
0.03
0.02
0.01
0.00
net axial force, $(p_x - \tau_x)/p_o$
0
1
2
throat
axial distance, x/w
exit
Maxwell, a=1.0
Maxwell, a=0.5
CLL (diffuse), a=0.5
CLL (orig), a=0.5

Fig. 10

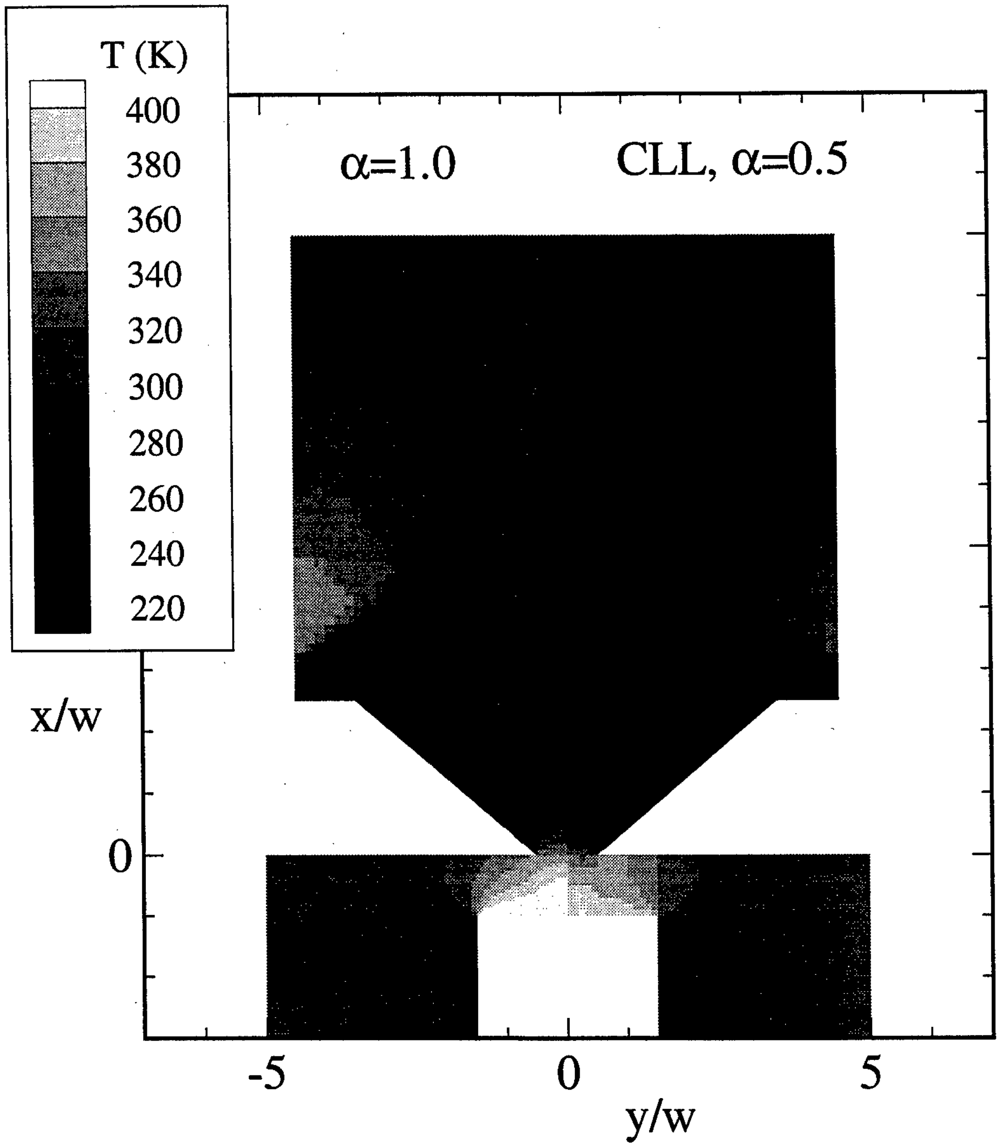
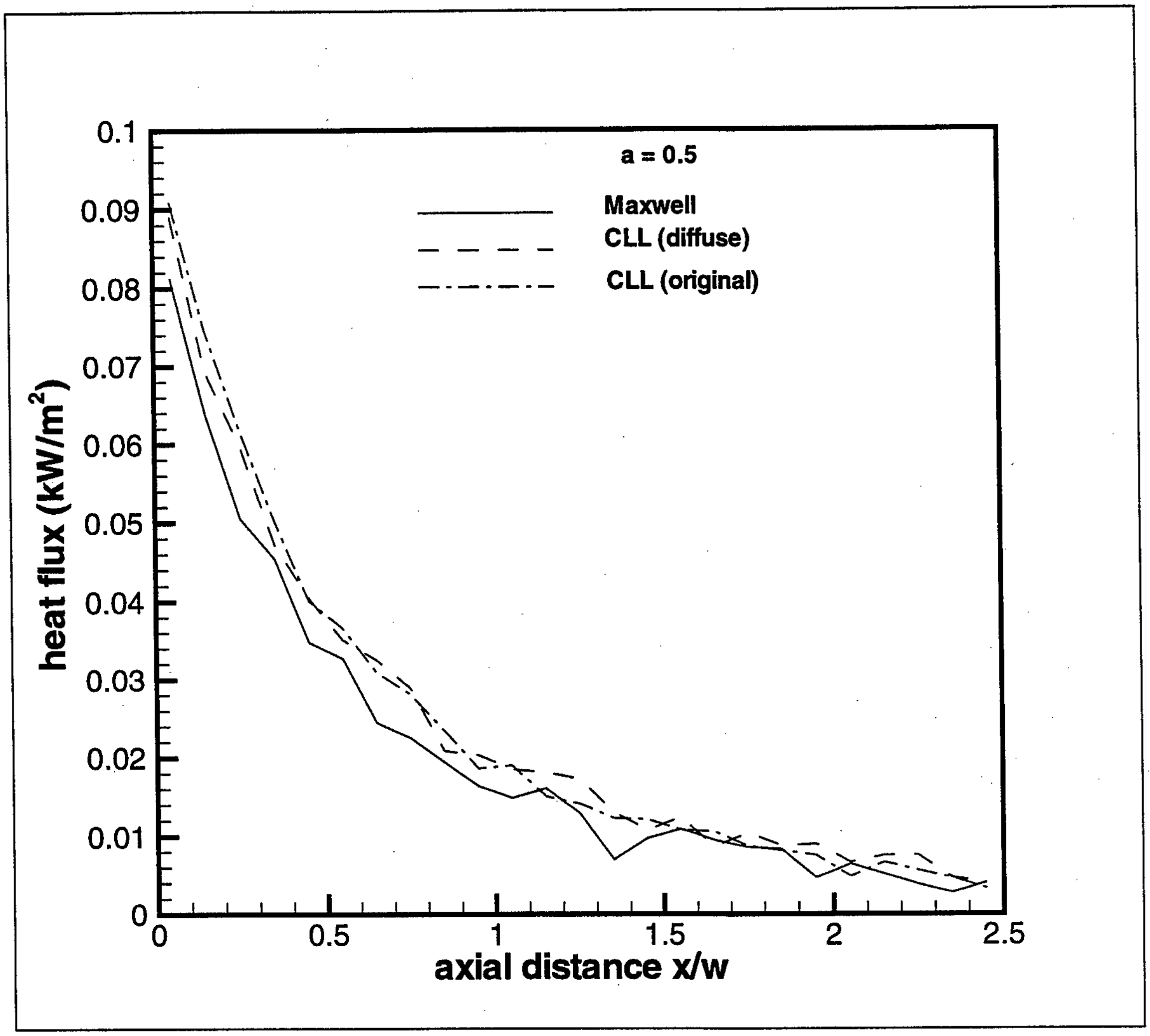
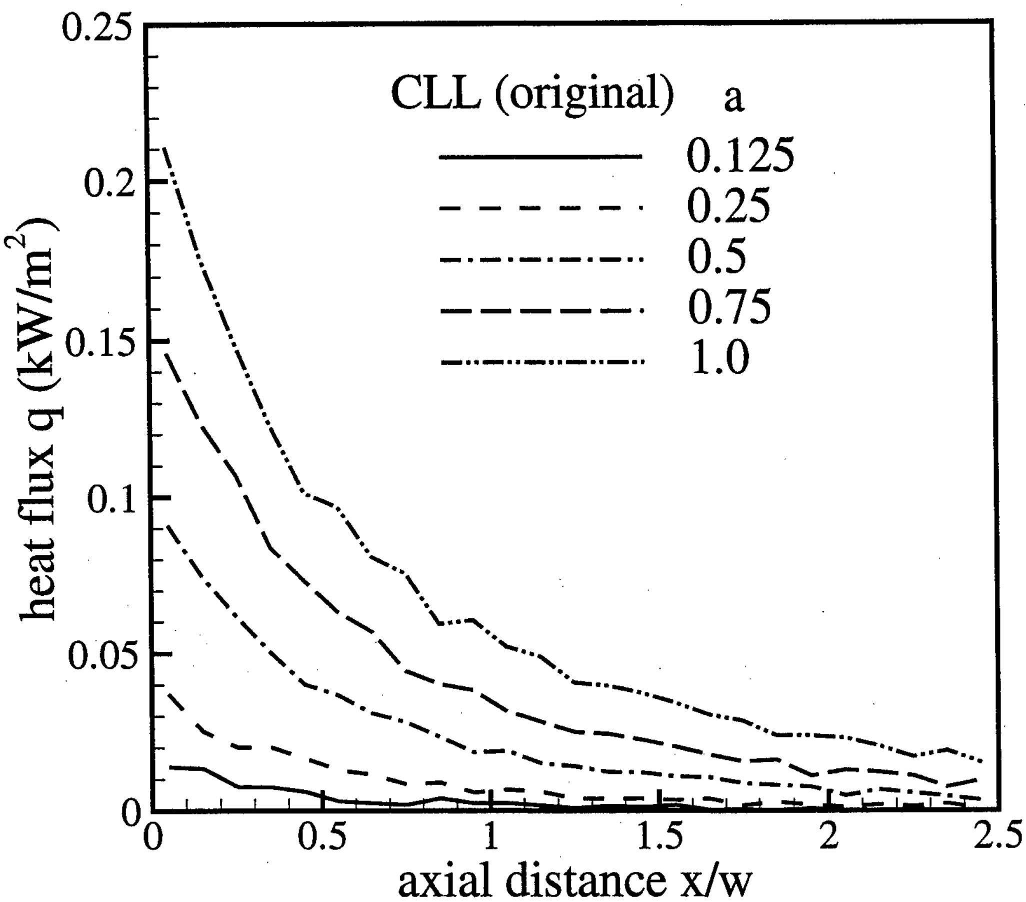


Fig. 11

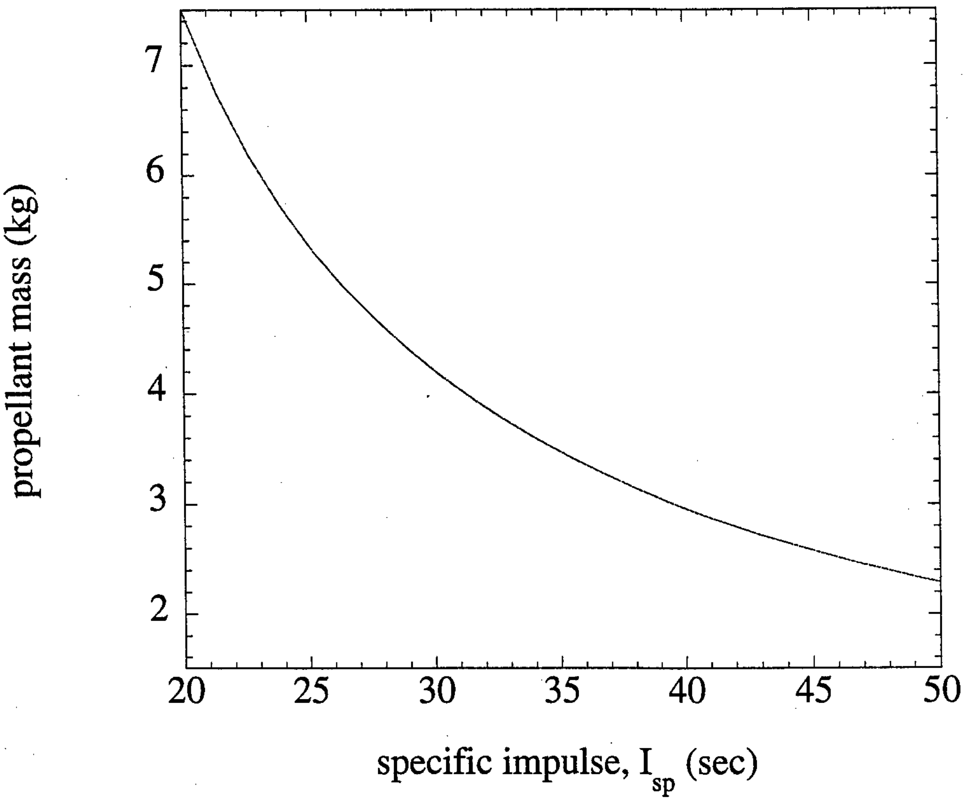


a = 0.5
Maxwell
CLL (diffuse)
CLL (original)
heat flux (kW/m²)
axial distance x/w
0
0.01
0.02
0.03
0.04
0.05
0.06
0.07
0.08
0.09
0.1
0
0.5
1
1.5
2
2.5

title


CLL (original) a
0.125
0.25
0.5
0.75
1.0
heat flux q (kW/m²)
axial distance x/w
0
0.05
0.1
0.15
0.2
0.25
0.5
1
1.5
2
2.5

title


propellant mass (kg)
7
6
5
4
3
2
20
25
30
35
40
45
50
specific impulse, I_{sp} (sec)

title